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THE INTERACTION OF He WITH A $\frac{1}{2}\langle 111\rangle\{110\}$ EDGE DISLOCATION IN W AND Mo

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The positions of the metal atoms around a $\frac{1}{2}\langle 111\rangle\{110\}$ edge dislocation in Mo and W are calculated using the Wilson–Johnson potentials. The boundary conditions are given by anisotropic elasticity theory. The He–metal potential, also developed by Wilson and Johnson, is used to calculate the position with maximum energy gain for a He-atom.

NUCLEAR-REACTOR TECHNOLOGY^{1,2} has given an impetus to several investigations carried out in order to obtain an understanding of the fundamental radiation damage phenomena in metals.

Experimental helium implantation studies were carried out by Kornelsen³ on the basis of measurements of the desorption spectra. For an analysis of these measurements it is necessary to understand the configurations of the defects and their binding energies to He in metals.

In calculations reported in the literature of the He–defect interactions, so far only He and (di-) vacancies have been considered. The purpose of the present communication is to report the results of the calculation of the energy of interaction of a He-atom with $\frac{1}{2}\langle 111\rangle\{110\}$ edge dislocation commonly found in b.c.c. metals.

The model consists of approximately 3000 atoms arranged in a b.c.c. crystal lattice containing a perfect edge dislocation with Burgers vector $\frac{1}{2}\langle 111\rangle$ lying on a $\{110\}$ plane. It is introduced into the crystallite by initially submitting each atom in it to the displacements predicted by anisotropic elasticity theory.

Once these positions have been determined it is assumed that the atoms will relax to their final positions under the influence of interatomic pairwise central forces resulting from the interaction potential. The positions of the boundary atoms were fixed during the relaxation procedure. The atomic configuration was determined using Gibson's integration procedure.⁴

The interatomic potentials for tungsten and molybdenum and the He–W and He–Mo interaction functions were derived by Johnson and Wilson.⁵ The He–metal interatomic potentials were calculated by the

modified Wedepohl method in the Hartree–Fock–Slater approximation to the exchange interaction. These potentials are repulsive at distances < 3.8 Å.

The metal–metal interaction function is repulsive at distances < 2.6 Å and cut-off at a radius of 3.8 Å.

We know from an earlier investigation that this dislocation is narrow, both in tungsten and in molybdenum, without any stacking fault. Some displacement occurs in the core region parallel to the dislocation line in the $\langle 112\rangle$ direction.⁶ The initial atomic positions in Mo possess already a displacement component in the $[112]$ direction based on anisotropic elasticity theory. The displacement in the $X_3(z)$ direction along the dislocation line can be written according to the procedure of Eshelby⁷ as:

$$U_3 = \operatorname{Re} \sum_n^3 \alpha(n) [\beta(n) \gamma(n) + 2s_{25}^t] \ln \left(\frac{x_1 + p_n x_2}{x_1 - p_n x_2} \right) \quad (1)$$

where

$$\beta(n) = (s_{25}^t s_{12}^t p_n^2 + 3s_{25}^t s_{22}^t + s_{23}^t s_{25}^t) \quad (2)$$

and s_{ij}^t represents the compliance relative to the orthogonal system with reference axes X_1 , X_2 and X_3 along the $[\bar{1}11]$, $[110]$ and $[\bar{1}1\bar{2}]$ directions, respectively. If the elastic constants correspond to the isotropic condition, both s_{25}^t and the displacement component U_3 are equal to zero. In the case of tungsten using the elastic constants given by Featherston and Neighbours⁸ these initial displacements were negligible.

After the atomic configuration of the present edge dislocation has been determined, the potential energy of a He atom was calculated for a grid of positions separated by steps of 0.3 Å within a small block around the dislocation core as is indicated in Fig. 1. The

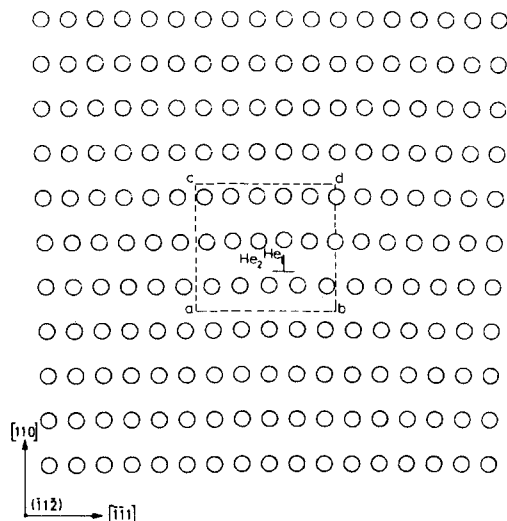


Fig. 1. The atomic configuration of one $(\bar{1}\bar{1}2)$ plane of the relaxed tungsten lattice containing an $\frac{1}{2}\langle 111 \rangle \{110\}$ edge dislocation. The potential energies of He atoms are calculated within the block outlined in the figure. He₁ and He₂ represent the projected distorted octahedral sites for which He possesses minimum potential energy (plane 6 in Fig. 2).

computational block contains six atomic layers in the $[\bar{1}\bar{1}2]$ direction because of the six planes periodicity along the dislocation line. The lattice has not been relaxed anew for each position because that would have cost too much computer time. The unrelaxed position of the atom possessing minimum potential energy was found in this way as illustrated in Fig. 1 by "He₁".

This unrelaxed site is also indicated in Fig. 2 which shows the projection on the (110) slipplane of the two atomic layers below the slipplane and the two layers above it for the dislocated lattice of tungsten.

The unrelaxed distorted octahedral sites *between* two $(\bar{1}\bar{1}2)$ atomic layers possess lower potential energy for the He atom than those *in* $(\bar{1}\bar{1}2)$ layer of atoms.

Relaxing the lattice anew containing the He atom at the octahedral site He₁ the total energy of the lattice E_{D+He_1} was calculated and compared with the total

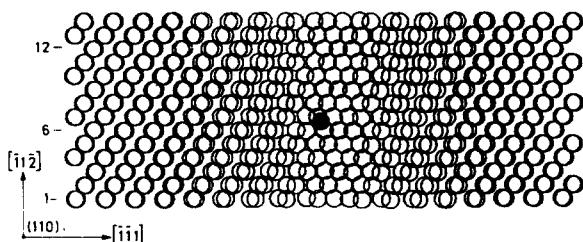


Fig. 2. The projection on the (110) slip-plane of the two atomic layers below the slip-plane and of the two layers above it for the dislocated tungsten lattice. The interstitial atom He₁ is shaded.

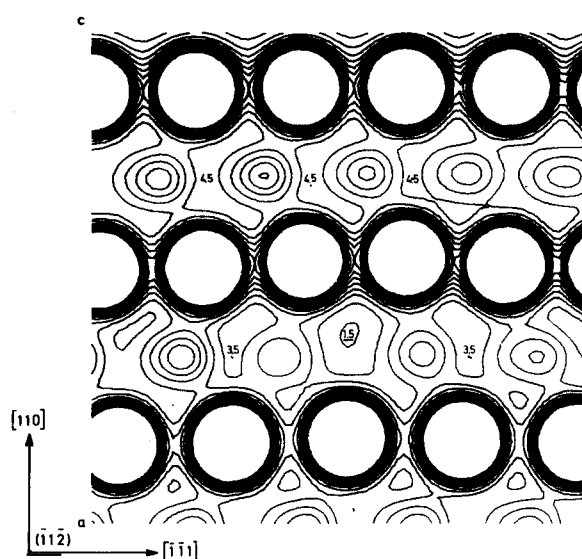


Fig. 3. The contour lines of equal potential energy for a helium atom in the dislocated molybdenum lattice. The location of the contour lines within the crystallite is indicated by a , b , c and d in Fig. 1. The contour lines are plotted for energies from 0.5 to 15 eV with intermediate steps of 1 eV.

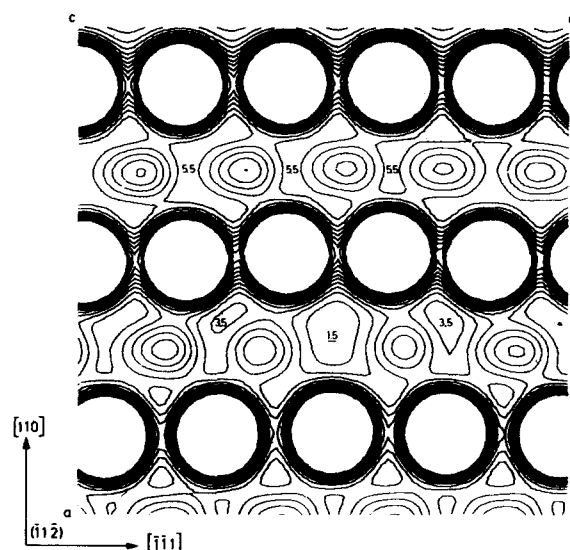


Fig. 4. The contour lines of equal potential energy for a helium atom in the dislocated tungsten lattice. The diagram is entirely analogous to Fig. 3.

energy of the relaxed atomic configuration without an He atom: E_D . During relaxation the He atom displaces itself in the $[\bar{1}\bar{1}2]$ direction over a distance of about 0.6 Å. The change in the configurational energy of the lattice by putting an He atom close to the dislocation line is then given by:

$$\Delta E_{He_1 D} = E_{D+He_1} - E_D. \quad (3)$$

Analogously, the changes in the configurational energies were calculated for a perfect Mo and W lattice containing an He atom at an octahedral site:

$$\Delta E_{\text{He},P} = E_{P+\text{He}_1} - E_P. \quad (4)$$

The earlier result of Wilson and Johnson, that the formation energy for a single He atom is minimal for the octahedral position was found to be confirmed.⁵ The values calculated for $\Delta E_{\text{He},D}$ and for $\Delta E_{\text{He},P}$ are 3.42 and 4.97 eV⁹ and 3.93 and 5.46 eV for molybdenum and tungsten, respectively. The values $\Delta E_{\text{He},P}$ are somewhat higher than the values obtained by Wilson and Bisson^{5,10} (4.91 and 5.44 eV).

For the binding energies of the He atom in the dislocated lattices for molybdenum and tungsten we found: 1.55 and 1.53 eV, respectively using the expression:

$$E_{B_1} = -(\Delta E_{\text{He},D} - \Delta E_{\text{He},P}) \quad (5)$$

If the saddle points of the binding energy for He between two adjoining octahedral sites is the tetrahedral site, the activation energy E_{He}^m for the migration in the perfect lattices of molybdenum and tungsten are found to be 0.3 and 0.24 eV, respectively. The determination of the migration energy in the crystallite containing the edge dislocation is a more difficult problem because of the disturbed symmetry around the dislocation. The nearest neighbour equilibrium position for a helium atom is indicated by He₂ in Fig. 1. If the path is chosen through the distorted tetrahedral site while the crystallite is allowed to relax in each step along the path, the migration energy is determined by the highest energetical threshold along this path. We determined the migration energy lying as being in the range of 0.3 until 0.4 eV for molybdenum and tungsten. There is, however, an uncertainty about the migration energy because the choice of the computational path is to some extent arbitrary.

The unrelaxed saddle points between the minima in the $[\bar{1}1\bar{2}]$ are higher than those in the $[\bar{1}11]$ direction. Figures 3 and 4 give the contour lines of equal potential energy for an He atom in molybdenum and tungsten. The contour lines were calculated for a relaxed crystal-

lite with an He atom originally present at the site for which He possesses minimum potential energy. For the calculation of the contour lines the He atom was moved within the block of Fig. 1 and are given for one $(\bar{1}1\bar{2})$ plane through the distorted octahedral site. The contour lines from 0.5 to 15 eV are plotted with intermediate steps of 1 eV. The regions with high potential energy represent the positions of the metal atoms above the present $(\bar{1}1\bar{2})$ plane which contains the distorted octahedral site for which He possesses minimum potential energy, and the positions of the metal atoms below this plane.

Consider the desorption of He from the dislocation-system as a dissociation reaction $\text{HeD} \rightarrow \text{He} + D$. The required dissociation energy $E_{\text{He},D}^{\text{dis}}$ is then given by:

$$E_{\text{He},D}^{\text{dis}} = E_{\text{He}}^f + E_D^f - E_{\text{He},D}^f + E_{\text{He}}^m \quad (6)$$

where E^f represents the formation energy relative to the perfect lattice. Assuming a migration energy of 0.4 eV we found for the dissociation energies 1.95 and 1.93 eV for molybdenum and tungsten, respectively.

These values are smaller than the dissociation energies of He associated with a single vacancy (4.2⁹ and 4.4 eV in molybdenum and tungsten, respectively).

The relatively high binding energy for the He vacancy-complex can be understood easily: more metal atoms are at greater distances from the He atom than in the case when He is placed at an octahedral site. The binding energy of He to a dislocation is essentially due to the missing half plane. However, the distances between the metal atoms and He in the relaxed dislocation do not differ much from those in the perfect system and the binding energy is lower than for He-vacancy complex assuming a repulsive He-metal interaction potential.

The possibility of helium aggregates around the $\frac{1}{2}\langle 111 \rangle\{110\}$ edge dislocation will be investigated. Helium clustering on (110) planes in the perfect lattice of molybdenum has been predicted.^{9,11}

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